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4. TITLE AND SUBTITLE			5. FUNDING NUMBERS
Fundamentals of friction and vapor phase lubrication. f49620-01-1-0069			
6. AUTHOR(S)			
Professor Andrew J. Gellman			
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION
Department of Chemical Engin	eering		REPORT NUMBER
Carnegie Mellon University			
Pittsburgh, PA 15213			•
9. SPONSORING/MONITORING AGENCY A	IAME(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING
USAF, AFRL			AGENCY REPORT NUMBER
AF Office of Scientific Research	ch		
4015 Wilson Blvd., Room 713			
Arlington, VA 22203-1954			
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION AVAILABILITY STATE	MENT		12b. DISTRIBUTION CODE
Approved for public release. D			
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<u>AFOSR - Final Report</u> <u>Fundamentals of Friction and Vapor Phase Lubrication</u>

Grant No. AFOSR-F49620-01-1-0069 Duration - Dec. 1, 2000 to April 30, 2004

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1. OBJECTIVES & ACCOMPLISHMENTS

This is the final report for the three year research program on "Fundamentals of Friction and Vapor Phase Lubrication" conducted at Carnegie Mellon with support from AFOSR grant number F49620-01-1-0069. The report summarizes the program objectives and summarizes the accomplishments and progress of the research towards the development of new methods for high temperature, vapor phase lubrication (VPL), understanding the tribological properties of quasicrystalline films and the development of a fundamental understanding of friction. The three primary objectives of the work have been:

- Exploration of a new approach to vapor phase lubrication of ceramics by surface activation with high vapor pressure Fe containing compounds such as Fe(CO)₅.
- Understanding the fundamental origins of friction anisotropy in crystalline metals and of lubrication of metal-metal interfaces.
- Probing the origins of the frictional properties of quasicrystalline surfaces through comparison with quasicrystalline approximants.

These objectives range from application-oriented to fundamental tribological science.

Our research has produced a number of important results over the course of the past 3+ years. The highlights are as follows:

- We have completed a proof of concept demonstration of the ability to activate ceramic surfaces for vapor phase lubrication. Fe has been deposited onto a SiC surface from the vapor phase by decomposition of Fe(CO)₅. This Fe has been shown to activate the surface and induce the subsequent decomposition of vapor phase tricresylphosphate (TCP) on the SiC surface to leave a film of carbon and phosphorus, as needed for vapor phase lubrication. The rates of film formation are accelerated by the presence of Fe and further accelerated by oxidation of the Fe film.
- A molecular level understanding has been developed of the decomposition mechanisms of arylphosphates, alkylphosphates, and alkylthiophosphate vapor phase lubricants on Fe surfaces.
- Friction anisotropy between metal single crystal surfaces has been explored. This anisotropy arises from anisotropy of the bulk mechanical properties of the single crystals. Our most recent work has corroborated the initial observations of friction anisotropy on Ni(100) by demonstrating the same phenomenon using Pd(100) surfaces.
- Careful comparison of the friction and oxidation properties of Al_xCu_yFe_z quasicrystals and approximants has shown that the properties are quite similar. This implies that bulk materials or Al_xCu_yFe_z thin films do not need to have uniform compositions lying within the rather narrow window of the quasicrystalline composition in order to have the tribological properties attributed to the quasicrystalline phases.

This work has been published in a number of scientific articles that have been published over the course of the grant period and will continue to be published during the coming year. One such review article summarizing several aspects of the work was recognized as the 'Best Paper of 2002' in the *Journal of Engineering Tribology*.

2. TECHNICAL PROGRESS

2.1 Vapor lubrication of ceramics

Ceramics such as SiC are not readily amenable to VPL because their surfaces are unreactive by comparison with those of most metals. As a result this limits their potential for use at the extremely high temperatures where VPL is the only viable method of lubrication. We have proposed and have explored a novel approach to the vapor lubrication of SiC. The idea has been to activate SiC surfaces via decomposition of high vapor pressure Fe containing compounds such as Fe(CO)₅. Vapor phase tricresylphosphate (TCP) is known to react on Fe surfaces at high temperatures to generate a lubricating film. If Fe deposited on the surface of SiC can catalyze the same decomposition reaction, then a lubricating film of carbon and phosphorus will be deposited onto the SiC surface. If both Fe and TCP are transported to ceramic surfaces through the vapor phase, then this lubricating film can be continuously replenished.

Demonstration of VPL of SiC surfaces has been performed by studying the surface chemistry of clean and Fe modified SiC surfaces in a surface analysis chamber that allows exposure of the surface to vapor phase lubricants. Our initial work modified the clean SiC surface by exposure to Fe(CO)₅ at temperatures in the range 400-800K. Auger spectroscopy was used to demonstrate that the Fe(CO)₅ decomposed to deposit Fe onto the SiC surface (Figure 1). The Fe deposition rate is clearly temperature dependent and is most efficient at T \sim 600K when using Fe(CO)₅ as the Fe source. The early work on this project demonstrated that while small model vapor lubricants such as (CH₃O)₃P will not decompose on the clean SiC surface they will decompose once the surface has been modified by the deposition of Fe from Fe(CO)₅ (Figure 1).

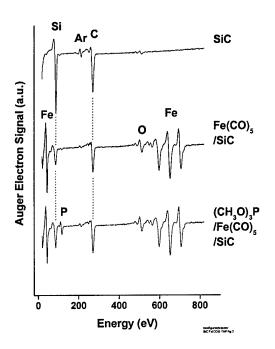


Figure 1. Auger spectra of the clean SiC surface, the surface after exposure to Fe(CO)₅, and the Fe modified SiC surface after exposure to (CH₃O)₃P. Fe(CO)₅ clearly deposits Fe onto the SiC surface and activates it for decomposition of organophosphorus compounds.

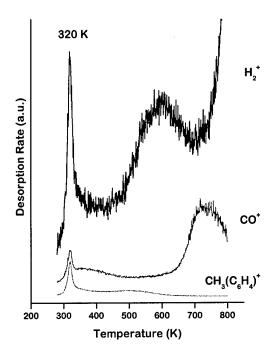


Figure 2. TPD of TCP on Fe modified SiC surface. The appearance of tolyl, H₂ and CO desorption products among others indicates that the TCP is decomposing on the surface. Auger spectroscopy reveals the deposition of P and C onto the surface as a result of TCP decomposition.

Most recently the SiC, Fe/SiC and oxidized Fe/SiC surfaces have been exposed to TCP vapor. TCP has been exposed to the SiC and Fe/SiC surfaces using a specially designed dosing apparatus that enables us to introduce very high molecular weight, low vapor pressure materials into the UHV chamber. Figure 2 shows the temperature programmed desorption (TPD) spectrum obtained from the Fe/SiC surface following exposure to TCP. The desorption of tolyl groups, H₂ and CO clearly reveals the decomposition of the TCP on the Fe modified surface. The most revealing experiments have been those using Auger Electron Spectroscopy (AES) to monitor the evolution of the surface composition during exposure to TCP (Figure 3). The peaks due to C and P grow while those due to Si and Fe are attenuated. Figure 4 compares the C and P film deposition rates on the clean SiC surface (open circles) with those on two surfaces modified by adsorbed Fe at different coverages (Fe/SiC = 0.2 and 0.9, red squares). These data clearly show that the presence of Fe activates the SiC surface and accelerates the deposition of the C and P film. Also shown in figure 4 are the C and P film growth rates on surfaces that have be activated with Fe and then oxidized (blue diamonds). Under the conditions used the oxide film has the stoichiometry FeO. Clearly, oxidation of the surface further activates the surface for TCP decomposition. This effect of Fe oxidation is consistent with prior work on the surface chemistry of TCP on Fe.

TCP decomposition on Fe activated SiC surfaces has been demonstrated over a wide range of temperatures (500 - 850 K). At all temperatures the presence of Fe on the SiC surface activated it for deposition of C and P films. Furthermore, Fe oxidation accelerates TCP decomposition. This data constitutes a compelling proof-of-concept demonstration that ceramic surfaces can be activated through the vapor phase for vapor lubrication by compounds such as TCP.

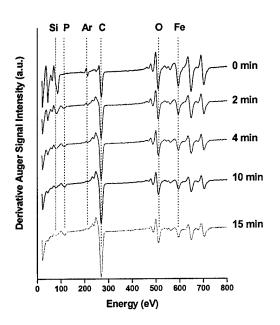


Figure 3. Auger spectra of the Fe modified SiC surface during exposure to TCP at 500 K. The Fe has been oxidized prior to exposure to TCP. The C and P peaks grow as the C&P film is deposited on the surface. The Si and Fe peaks are attenuated by the C&P film growing over them.

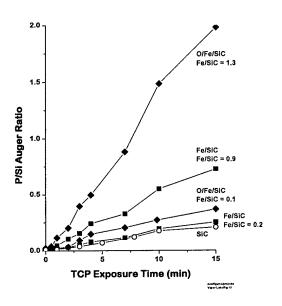


Figure 4. Growth of the P/Si Auger peak ratio during exposure of TCP to SiC surfaces at 500 K. The open circles (o) show some deposition onto the clean SiC surface. The deposition rate is enhanced on surfaces modified by Fe (red squares, I). Oxidation of the Fe accelerates the deposition of P even further (blue diamonds, •). Note that the C/Si ratio exhibits the same trends.

2.2 TCP decomposition mechanism on Fe surfaces

The surface chemistry of vapor phase lubricants occurs by a very complex mechanism that leads from adsorption of molecules such as TCP to the formation of lubricating films containing carbon and phosphorus. These reactions are clearly catalyzed by the surface itself and the rates of film deposition are dependent on the surface. One of the goals of the research has been to understand the nature of the initial steps in the reaction mechanism. Three compounds have been studied in the course of the work: tricreylphosphate ((CH₃C₄H₄O)₃P=O), tributylphosphate ((C₄H₉O)₃P=O), and tributylthiophosphate ((C₄H₉O)₃P=S). The interesting feature of these studies is that mechanism of their decomposition on the Fe surface is dependent on the nature of the ligands on the central phosphorus atoms. The three compounds have been adsorbed on the Fe surface at low temperature under UHV conditions and then heated to induce decomposition and the desorption of reaction products. The reaction products have been detected using mass spectrometry. Previous work in our laboratory has shown that the ability of these compounds to decompose and deposit carbon onto the surface is a key feature of their ability to function as vapor phase lubricants. The aryl phosphates such as TCP work well because their ligands have no β-CH bonds. As a consequence, when they decompose the ligands decompose almost completely to deposit significant amounts of carbon on the surface. This appears to be critical to the function of the vapor phase lubricant.

Recent work has revealed interesting differences between the surface chemistries of tributylphosphate ($(C_4H_9O)_3P=O$), and tributylthiophosphate ($(C_4H_9O)_3P=S$). The tributylphosphate decomposes by dissociation of the C-O bonds to deposit butyl groups on the surface. These then react by β -hydride elimination to yield butene in the gas phase. In contrast the tributylthiophosphate decomposition results in the appearance of butanal in the gas phase. This indicates that in tributylthiophosphate the P=S bond dissociates initially. This leads to the formation of adsorbed tributylphosphite ($(C_4H_9O)_3P$) which then dissociates by decomposition of the P-O bonds leading to the formation of adsorbed butanoxy groups. These then undergo β -hydride elimination to yield butanal. The last steps in this process are identical to those observed using trimethylphosphite ($(CH_3O)_3P$).

2.3 Friction anisotropy between fcc(100) surface

Fundamental studies of friction between well-defined surfaces have been an integral part of this research program. One of the fundamental issues that we have addressed is that of friction anisotropy between crystalline surfaces. Friction anisotropy is the dependence of friction on the orientations of the lattice vectors of the two surfaces in contact with one another. One of our most interesting observations has been made between a pair of Ni(100) surfaces which were oriented at different angles with respect to one another prior to contact and friction measurements. That work revealed friction anisotropy in the sense that the friction was minimized when the two surfaces lattices were rotated by 45° with respect to one another. Furthermore, this anisotropy was still observed in the presence of adsorbed sulfur atoms and in the presence of ethanol adsorbed at coverages up to 4 monolayers.

The sliding contact of two metal surfaces under macroscopic loads always results in the plastic deformation of the surfaces in the contact region. The implication of our observations of friction anisotropy is that it arises as a result of the bulk plastic deformation properties of the Ni rather than the commensurate or incommensurate contact of surface lattices. As such the same anisotropy ought to be observable between other fcc(100) surfaces in contact with one another.

During this grant period we have made a series of friction measurements between Pd(100) surfaces brought into contact at various different azimuthal orientations. Both Ni and Pd have fcc bulk structures and thus these measurements ought to yield the same anisotropy as was observed between the Ni(100) surfaces. Figure 5 shows the friction between two Pd(100) surfaces with 4 monolayers of octane on each as a function of the misorientation angle. Figure 5 clearly shows that there is a minimum in the friction at a misorientation angle of 45°. This minimum also occurs for an angle of 135° which is equivalent by symmetry to the 45° misorientation. The principle point to be made is that this most recent work with the Pd(100) surfaces has reproduced the same friction anisotropy as was observed using Ni(100) surfaces. This indicates that the phenomenon is probably a general property of the fcc lattice.

2.4 Adsorbate effects on friction

Past work with the UHV tribometer has explored the effects of adsorbed species on the frictional properties of Cu(111) and Ni(100) surfaces. This work has made use of several alcohols including ethanol and trifluoroethanol as the adsorbates. One of the principle observations of that work has been that at coverages less than one monolayer the adsorbed alcohols have no observable effect on the friction between the surfaces. As the coverage is increased, however, lubrication or a reduction in friction is observed once the coverages increase past one monolayer.

During the course of our study of the friction between Pd(100) surfaces we have made measurements as a function of the coverage of adsorbed octane. Octane was chosen as the

Friction Coefficient vs. Lattice Misorientation 4 ML Octane/Pd(100)

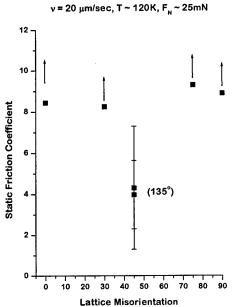


Figure 5. Friction coefficients between pairs of Pd(100) surfaces with 4 monolayers of octane. The friction coefficient is unmeasurably high at angles other than 45° (and 135°). This friction anisotropy is also observed at higher octane coverages and is identical to that observed between Ni(100) surfaces.

Friction Coefficient vs. Coverage Octane/Pd(100) @ 45°

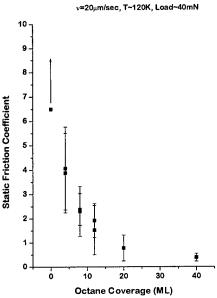


Figure 6. Friction versus octane coverage for interfaces between Pd(100) surface. The decrease of friction with increasing octane coverage is much slower than for the Ni(100) and Cu(111) surface modified by alcohol adsorption.

lubricant because it will adsorb and desorb reversibly from the Pd(100) surface. As such its coverage can be calibrated quite easily using temperature programmed desorption methods. Figure 6 shows the values of friction coefficients measured between the Pd(100) surfaces as a function of octane coverage with the surface lattices held at a misorientation angle of 45°. It is immediately obvious that the dependence of friction on octane coverage is much different from that observed using the alcohols. The friction coefficient decreases much less rapidly than was observed with the alcohols on Cu(111) and Ni(100) surfaces. In measurements in which the coverage has been varied in fairly small increments around 0-2 monolayers there is no discernable discontinuity in the friction at one monolayer coverage. This was a clear feature of the experiments performed with the alcohols on Cu(111) and Ni(100) surfaces. These new results using adsorbed octane indicate that the dependence of friction on lubricant coverage is influenced strongly by the nature of the lubricant.

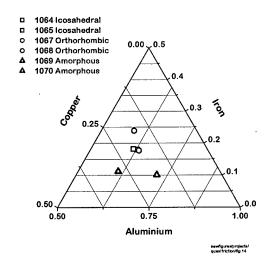
2.5 Quasicrystal tribology

Quasicrystals have a number of unique and potentially important properties, some of which may be directly associated with their ordered but aperiodic structure. One of these properties is nominally low friction. The only measurements of the intrinsic frictional properties of interfaces between highly characterized and truly clean surfaces of quasicrystals have been made in my laboratory over the past few years. These have shown that the frictional properties of truly clean quasicrystalline surfaces are significantly higher than those of air-exposed surfaces. In addition controlled oxidation of the surfaces has shown that the lower friction observed in air is due in part to the presence of a thin oxide film on the quasicrystalline surface.

Over the past two years a comprehensive set of tribological and materials properties measurements have been made using a set of thin Al_xCu_yFe_z films having compositions that lie within and around the quasicrystalline region of the compositional phase diagram. The set of samples were prepared by TA&T Inc. using sputter deposition and have been characterized extensively by other collaborating research groups around the country. The sample surfaces were cleaned by Ar⁺ ion sputtering and annealing treatments in order to generate well-characterized surfaces prior to measurement of their tribological properties. Most importantly, the extended annealing treatments used to generate the crystalline and quasicrystalline phases in these materials were performed in UHV (10⁻⁹ Torr) to eliminate any potential for oxidation of the surfaces or the bulk during the annealing process.

The compositions of the $Al_xCu_yFe_z$ films were first determined using x-ray photoemission spectroscopy and all were found to have compositions that lie in and around those of the quasicrystalline region of the compositional phase diagram. Analysis of the x-ray diffraction patterns obtained from the six samples revealed that following annealing treatments two of the samples contained the quasicrystalline icosahedral phase, two contained a crystalline orthorhombic approximant phase and two remained amorphous. The compositions and the structures of the six samples are shown in figure 7. These samples have provided us with an excellent opportunity to probe the tribological properties of a set of materials with similar bulk compositions but varying crystalline or quasicrystalline order.

Friction has been measured between the surfaces of pairs of the quasicrystalline films using an UHV tribometer that is unique to my laboratory. This has enabled us to measure the intrinsic frictional properties of clean $Al_xCu_yFe_z$ surfaces and oxidized surfaces. Friction coefficients were measured multiple times using fresh contacts between previously untouched surfaces. The contact and sliding conditions were: $F_N = 60$ mN, $\nu_s = 10$ μ m/s, and T = 300K. Figure 8 shows



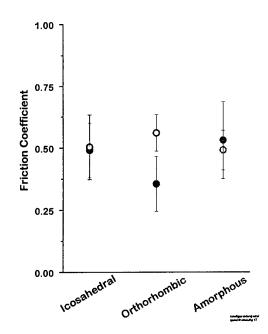


Figure 7. Compositional phase diagram for the $Al_xCu_yFe_z$ alloy system. The compositions of the alloys used in this work lie in and around the quasicrystalline region.

Figure 8. Friction coefficients measured between pairs of the six $Al_xCu_yFe_z$ alloy films. Friction coefficients did not vary significantly among the six in spite of the fact that the structures include quasicrystal, crystal, and amorphous. $F_N = 60$ mN, $v_s = 10$ μ m/sec, T = 300K.

that the friction coefficients do not differ significantly among the six samples. Although differences were observed between the friction coefficients of the $Al_xPd_yMn_z$ quasicrystal and the $Al_xPd_yMn_z$ approximant these are not apparent in the $Al_xCu_yFe_z$ alloy system.

The final conclusions of the work performed to date on the $Al_xCu_yFe_z$ quasicrystals and their approximants are that the tribological properties are not critically sensitive to the bulk structure. On the one hand this suggests that the low friction coefficients measured in air by other groups studying the quasicrystals are not intrinsically related to the quasicrystalline structure. From an applications perspective this is probably a positive feature since the quasicrystalline region of the compositional phase diagram for the $Al_xCu_yFe_z$ alloy system is so small. Practically, it would be quite difficult to prepare thin sputtered $Al_xCu_yFe_z$ films with compositions that fall reproducibly within the fairly narrow quasicrystalline region.

2.6 MEMS Tribology

The final work initiated during the grant period was an initial study of the feasibility MEMS lubrication by vapor phase methods. The interstices of MEMS devices include long, narrow channels with high aspect ratios. It is not clear that vapor lubricants could diffuse into the interstices of such devices rapidly enough to support the wear of surfaces that are remote from the exterior of the device or the source of the vapor lubricant. We have developed a fairly simple model of MEMS lubrication which describes the diffusive, gas phase transport of the vapor lubricant down the channel and its consumption along the length of the channel by wear processes occurring on the surface of the MEMS device. The theory indicates that over a wide range of conditions the relationship between the width of the channel, h, and the length of the channel, l, is given by the expression

$$l^2 \approx \frac{N_A P_0}{RTS} \cdot \frac{Dh}{k_w}$$
.

The quantities in this expression are Avagadro's number, N_A , the vapor pressure of the lubricant, P_0 , the gas constant, R, the absolute temperature, R, the density of adsorption sites on the surface, R, the gas phase diffusion constant, R, and the rate constant for the surface wear process, R. Most of these have a narrow range of possible values leaving R0 and R1 as the critical variables. For reasonable values of the lubricant vapor pressure and wear rates constants as high as 1 monolayer per second the allowable aspect ratio can be as high as R1 R1 indicates that provided one identifies a vapor phase lubricant with the correct surface chemistry, vapor phase lubricant is in fact amenable to use with MEMS devices.

2.7 Instrumentation

During the grant period we have made a number of major improvements to the instrumentation in my laboratory that should have a significant impact on our future studies of tribology and lubricant surface chemistry. One new apparatus has been constructed that will include a new UHV tribometer for use in our studies of friction between solid-solid interfaces. This chamber has instrumentation for surface preparation and surface analysis and will house a new UHV tribometer. We have installed a new surface analysis chamber with instrumentation for high resolution electron energy loss spectroscopy (HREELS). This contains a modern HREELS spectrometer which has the level of resolution needed to be able to examine the vibrational spectra of large complex molecules such as TCP vapor phase lubricants. One of our UHV surface analysis chambers has been equipped with a monochromated x-ray source that allows us to take much higher resolution x-ray photoemission spectra than is possible with conventional x-XPS instrumentations. Again this is needed for the studies of complex lubricants.

During the past six months we have been making major modifications to one of our UHV tribometers to allow us to make measurements of friction between surfaces in elastic contact. As mentioned in section 2.2 metal surfaces in sliding contact always undergo plastic deformation. From a fundamental perspective this always complicates the process that one is trying to understand. To address this we have built the prototype of a UHV tribometer that will allow us to measure friction between solid surfaces in elastic contact. This is based on the use of ultrathin Si(100) foils that can bend elastically when brought into contact with one another. Figures 9 & 10 show the Si foil and the prototype of this new tribometer.

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Figure 9. Si(100) foil bent into cylinder and mounted in a sample holder to go onto the UHV tribometer.

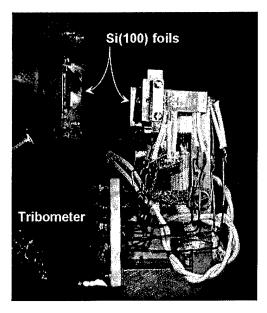


Figure 10. Prototype UHV tribometer. Si(100) foil samples have been mounted in a crossed cylinder geometry for preliminary friction measurements.

3. PERSONNEL

P.I.	9%
Postdoc	100%
Grad. Student	100%
Grad. Student	100%
Grad. Student	100%
	Postdoc Grad. Student Grad. Student

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- D. Kim, A.J. Gellman "Vapor phase activation of SiC surfaces for TCP decomposition" in preparation
- * these papers acknowledge AFOSR support for instrumentation used in those studies

5. INTERACTIONS / TRANSITIONS

5a. Conferences

- D. Sung, A.J. Gellman "A Comparison Study of Alkyl- and Aryl-phosphate Vapor Phase Lubricant Chemistry", AVS IMCTFC, San Diego, CA Apr. 2002
- D. Sung, A.J. Gellman "Surface Reaction Mechanisms of Organophosphate Vapor Phase Lubricants" AIChE Annual Meeting, Indianapolis, IN Nov. 2002
- C. Mancinelli, A.J. Gellman "Frictional Anisotropy at Crystalline Interfaces" ChEGSA Symposium, Pittsburgh, PA Nov. 2002
- C. Mancinelli, A.J. Gellman "Frictional Anisotropy at Crystalline Interfaces" FACSS Meeting, Baltimore, MA-Nov. 2002
- C. Mancinelli, A.J. Gellman "Frictional Anisotropy at Crystalline Interfaces" AVS Meeting, Denver, CO Nov. 2002
- D. Sung, A.J. Gellman "Surface Reaction Mechanisms of Organophosphate Vapor Phase Lubricants" AIChE Meeting, Indianapolis, IN Nov. 2002
- A.J. Gellman "Frictional properties of crystalline and quasicrystalline surfaces" Dept. of Materials Sci., Univ. of Pittsburgh, PA Feb. 2003
- A.J. Gellman "Friction anisotropy at crystalline interfaces" AVS Meeting, Baltimore, ML Nov. 2003
- A.J. Gellman "Friction anisotropy at crystalline interfaces" Univ. S. Carolina, Nov. 2003
- A.J. Gellman "Energetics of Oligomeric Lubricant Desorption from Surfaces" San Luis III Symposium, Merida, Venezuela March 2004

5c. Transitions

Seagate Technology, Inc. Research in tribological problems at the head-disk interface of magnetic storage devices is being conducted in my laboratory with support of Seagate.

National Storage Industries Consortium (NSIC). Research is supported in the P.I.'s lab on some fundamental issues in the lubrication of hard disk surfaces.

6. MAJOR ACCOMPLISHMENTS

- We have completed a proof of concept demonstration of the ability to activate SiC surfaces for vapor phase lubrication. Fe has been deposited onto a SiC surface from the vapor phase has been shown to activate the surface and induce decomposition of vapor phase tricresylphosphate (TCP).
- We have demonstrated the existence of friction anisotropy between metal single crystal surfaces by showing that the friction between the two surfaces depends on the orientation of their lattice vectors. The initial demonstration was made using Ni(100) surfaces. Our most recent work has corroborated the initial observations of friction anisotropy by demonstrating the same phenomenon with Pd(100) surfaces.
- Careful comparison of the friction and oxidation properties of $Al_xCu_yFe_z$ quasicrystals and approximants has shown that the properties are quite similar. This implies that bulk materials or $Al_xCu_yFe_z$ thin films do not need to have uniform compositions lying within the rather narrow window of the quasicrystalline composition in order to have the tribological properties often attributed to the quasicrystalline phases.

7. AWARDS and HONORS

Promoted to Department Head of Chemical Engineering at Carnegie Mellon University - Jan. 1, 2003.

Best paper of 2002, Journal of Engineering Tribology